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Two-Dimensional Classical Representations of the Partition Function of the Spin-1/2 Chain

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Starting from the Trotter formula, we derive several classical representations of the partition function of a spin-1/2 chain. We investigate the rate of convergence of the different approximants by means of exact calculations for small systems. We demonstrate that it is important to use approximants that have the same symmetry properties as the original quantum model.

I. Introduction

Recently, it has been shown that several mappings of the partition function of a d-dimensional quantum spin-1/2 model onto $(d+1)$-dimensional classical models [1, 2] exist and similar results have been derived for fermion lattice models [3–6]. In specific cases, these maps lead to the well-known Feynman path integral formulation of quantum statistical mechanics. This correspondence relates ground state properties of the $1-d$ Ising model in a transverse field [1, 7] and the $1-d$ XY model [8] to the thermodynamic properties of a $2-d$ Ising model. Furthermore, this equivalence opens the possibility of using powerful computational techniques developed for classical statistical mechanics in order to obtain information on the quantum model [4–6, 9].

A convenient way to obtain a classical representation for the partition function of the quantum model described by the Hamiltonian

$$H=\sum_{l=1}^{k} A_l \tag{1.1}$$

is to start from the Trotter formula [10, 11]

$$Z\equiv \mathrm{Tr}\exp(-\beta H)=\lim_{m\to\infty} Z_m \tag{1.2a}$$

where

$$Z_m\equiv \mathrm{Tr}\left[\exp\left(-\frac{\beta A_1}{m}\right)\ldots\exp\left(-\frac{\beta A_k}{m}\right)\right]^m. \tag{1.2b}$$

In practical applications, the only requirement on the choice of the operators A_l is that it is easy to find all eigenvalues and eigenvectors of each A_l.

The classical representation is then obtained by inserting complete sets of states (resolutions of the identity) in the expression (1.2b).

The basic idea of this approach is to study the convergence of Z_m as a function of m.

Except for some rigorous inequalities [11, 12] (which turn out to be of limited value in practical applications), only little is known about the nature of the approximation (1.2) and the effect of taking different decompositions (1.1).

In this paper we discuss the results of this approach applied to the $1-d$ spin-1/2 chain described by the Hamiltonian

$$H=-J_1\sum_i(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y)-J_3\sum_i\sigma_i^z\sigma_{i+1}^z-h\sum_i\sigma_i^z \tag{1.3}$$

where σ_i^α denote the Pauli spin matrices on site i.

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We will consider both free and periodic boundary conditions. The properties of this model have been discussed extensively and its behavior is well understood [13, 14].

Because this paper emphasizes the computational aspects rather than new physics, we will confine ourselves to small systems such that an exact (numerical) calculation of Z_m can be performed and a comparison with results obtained by diagonalizing the full Hamiltonian (1.3) can be made.

A similar study for the $1-d$ fermion model related to the model (1.3) can be found in [5].

In our opinion, this kind of work has to be done before one calculates the properties of large system. As it is unlikely that such calculation can be done without a Monte Carlo algorithm the information obtained from the study of small systems can be used to provide meaningful criteria for selecting a particular Monte Carlo scheme.

The plan of the paper is as follows. In Sect. 2 we take two slightly different decompositions for the model with free boundary conditions. In Sect. 3 we deal with periodic boundary conditions and in Sect. 4 we discuss some analytic results for the simplest approximations. Our conclusions are given in Sect. 5.

II. Free Boundary Conditions

A. Real Space Decomposition (RSD)

The simplest classical representation is found by decomposing the Hamiltonian in local two-site Hamiltonians [1]. In particular we take $k=N$ and

$$A_i=H_{i,i+1}\equiv -J_1(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y)-J_3\sigma_i^z\sigma_{i+1}^z -\frac{h}{2}(\sigma_i^z+\sigma_{i+1}^z). \tag{2.1}$$

In the following the ket $|S_i\rangle$ denotes the state where the spin on site i is up ($S_i=1$) or down ($S_i=-1$). A matrix element of $\exp\left(-\frac{\beta H_{i,i+1}}{m}\right)$ is given by

$$\langle S_i S_{i+1}|\exp\left(-\frac{\beta H_{i,i+1}}{m}\right)|S_i' S_{i+1}'\rangle =\delta_{S_i,S_i'}\delta_{S_{i+1},S_{i+1}'}T_1(S_i,S_{i+1}') +(1-\delta_{S_i,S_i'})(1-\delta_{S_{i+1},S_{i+1}'})T_{-1}(S_i,S_{i+1}'). \tag{2.2a}$$

Here $T_1(S,S')$ and $T_{-1}(S,S')$ have the matrix representation

$$T_1(S,S')=\tfrac{1}{4}(1-S\quad 1+S)\begin{pmatrix}a & b\\ b & d\end{pmatrix}\begin{pmatrix}1-S'\\ 1+S'\end{pmatrix}, \tag{2.2b}$$

$$T_{-1}(S,S')=c\,\delta_{S,S'}, \tag{2.2c}$$

and

$$a=\exp\left[\frac{\beta}{m}(J_3-h)\right] \tag{2.2d}$$

$$b=\exp\left(-\frac{\beta J_3}{n}\right)\cosh\left(\frac{2\beta J_1}{m}\right), \tag{2.2e}$$

$$c=\exp\left(-\frac{\beta J_3}{m}\right)\sinh\left(\frac{2\beta J_1}{m}\right), \tag{2.2f}$$

$$d=\exp\left[\frac{\beta}{m}(J_3+h)\right]. \tag{2.2g}$$

If we denote

$$\phi_{ij}=\prod_{l=1}^{i}S_{lj}S_{lj+1};\qquad \phi_{0j}=1,\ j=1,\ldots,m \tag{2.3}$$

application of Eq. (2.2a) gives

$$\langle S_{1j}\ldots S_{N+1j}|\exp\left(-\frac{\beta H_{12}}{m}\right)\ldots \cdot\exp\left(-\frac{\beta H_{NN+1}}{m}\right)|S_{1j+1}\ldots S_{N+1j+1}\rangle =\delta_{\phi_{N+1j},1}\prod_{i=1}^{N}T_{\phi_{ij}}(\phi_{i-1j}S_{ij},\phi_{ij}S_{i+1j}) \tag{2.4}$$

and the m-th approximant to the partition function reads

$$Z_m^{\mathrm{RSD}}=\sum_{\{S_{ij}\}}\prod_{j=1}^{m}\delta_{\phi_{N+1j},1}\prod_{i=1}^{N}T_{\phi_{ij}}(\phi_{i-1j}S_{ij},\phi_{ij}S_{i+1j}). \tag{2.5}$$

Note that because of the trace operation, we have to fulfil the requirement $S_{ij}=S_{ij+m}$, $\phi_{ij}=\phi_{ij+m}$, i.e. periodic boundary conditions in the new (Trotter) dimension. In the following, we will implicitly assume periodic boundary conditions in the Trotter direction.

Analytic results for $m=1$ are given in Sect. 4.

We may interpret (2.5) in terms of a $2-d$ Ising-like model but the string variables (2.3) introduce a strange kind of coupling between different rows and columns.

The decomposition (2.1) has been introduced by Suzuki [1, 15]. We have used (2.2a) to sum out intermediate states that appear at the left hand side of (2.4).

In Suzuki's formulation one has to sum over $2^{(N+1)(2m-1)}$ states whereas in our formulation one sums over $2^{(N+1)m}$ states and this is important in actual calculations because it reduces computer time.

Because this and the following two decompositions do not alter the symmetry in spin space, the sum in

(2.5) can be taken in subspaces of equal magnetization thereby eliminating the condition $\delta_{\phi_{N+1j},1}$.

B. Checker Board Decomposition (CBD)

An apparently different formula for Z_m is obtained by taking [2] $k=2$ and

$$A_1=\sum_{i=0}^{N/2-1} H_{2i+1,2i+2} \tag{2.6a}$$

$$A_2=\sum_{i=1}^{N/2} H_{2i,2i+1}, \tag{2.6b}$$

where we assume that N is even. Then (1.2) yields

$$Z_m^{\mathrm{CBD}}=\mathrm{Tr}\left[\exp\left(-\frac{\beta H_{1,2}}{m}\right)\exp\left(-\frac{\beta H_{3,4}}{m}\right)\cdots\right.$$
$$\cdot\exp\left(-\frac{\beta H_{N-1,N}}{m}\right)\exp\left(-\frac{\beta H_{2,3}}{m}\right)\exp\left(-\frac{\beta H_{4,5}}{m}\right)\cdots$$
$$\left.\cdot\exp\left(-\frac{\beta H_{N,N+1}}{m}\right)\right]^m. \tag{2.7}$$

Note that the only difference between this and the previous formulation is the order of the operators $\exp\left(-\frac{\beta H_{i,i+1}}{m}\right)$. A typical matrix element reads

$$\langle S_{1j}\cdots S_{N+1j}|\exp\left(-\frac{\beta A_1}{m}\right)$$
$$\cdot\exp\left(-\frac{\beta A_2}{m}\right)|S_{1j+1}\cdots S_{N+1j+1}\rangle$$
$$=\sum_{\{\hat{S}_{ij}\}}\langle S_{1j}\hat{S}_{2j}|\exp\left(-\frac{\beta H_{1,2}}{m}\right)|S_{1j+1}\hat{S}_{2j}\rangle$$
$$\cdot\ \langle S_{3j}S_{4j}|\exp\left(-\frac{\beta H_{3,4}}{m}\right)|\hat{S}_{3j}\hat{S}_{4j}\rangle\cdots$$
$$\cdot\ \langle S_{N-1j}S_{Nj}|\exp\left(-\frac{\beta H_{N-1,N}}{m}\right)|\hat{S}_{N-1j}\hat{S}_{Nj}\rangle\cdots$$
$$\cdot\ \langle\hat{S}_{2j}\hat{S}_{3j}|\exp\left(-\frac{\beta H_{2,3}}{m}\right)|S_{2j+1}S_{3j+1}\rangle\cdots$$
$$\cdot\ \langle\hat{S}_{Nj}S_{N+1j}|\exp\left(-\frac{\beta H_{N,N+1}}{m}\right)|S_{Nj+1}S_{N+1j+1}\rangle. \tag{2.8}$$

This expression has been used to relate $Z_m^{(2)}$ to the partition function of a modified $2-d$ eight-vertex model [2] and it also has an interpretation in terms of a $2-d$ spin model with a checkerboard-like lattice structure (see Fig. 1).

We now show that $Z_m^{\mathrm{RSD}}=Z_m^{\mathrm{CBD}}$. First we use (2.2a) to express Z_m^{CBD} in terms of $T_{\pm 1}$ and a change of variables then completes the proof.

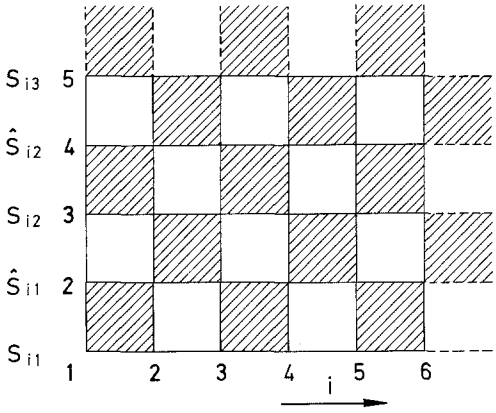

Fig. 1. Graphical interpretation of the approximation Z_m^{RSD} obtained from the representation (2.8). Only spins on the edges of a shaded square interact with each other. The sum over all $\hat{S}_{ij}$ can be carried out analytically

We have

$$Z_m^{\mathrm{CBD}}=\sum_{\{S_{ij}\}}\prod_{j=1}^{m}\delta_{\phi_{N+1j},1}\prod_{i=1}^{N/2}T_{\phi_{2i-1j}}(S_{2i-1j},\phi_{2i-1j}S_{2ij})$$
$$\cdot\,T_{\phi_{2ij}}(\phi_{2i-1j}S_{2ij},S_{2i+1j+1}). \tag{2.9}$$

For $m=1$, $\phi_{i1=1}$ and we have $Z^{\mathrm{RSD}}=Z^{\mathrm{CBD}}$. For $m>1$ we take $n=3$ and change variables $S_{nj+1}=\phi_{n-1j}S'_{nj}$, $S_{lj}=S'_{l,j-1}$ for $l>n$.

This leads to $\phi_{nj}=\phi'_{nj-1}$, $\phi_{lj}=\phi'_{lj-1}$ for $l>n$ where

$$\phi'_{ij}\equiv\prod_{l=1}^{i}S'_{lj}S'_{lj+1} \tag{2.10}$$

Now we may drop the primes and repeat the procedure for $n=5,7,\ldots$ and finally one observes that $Z_m^{\mathrm{CBD}}=Z_m^{\mathrm{RSD}}$.

Thus we have shown that both decompositions will give the same results for the thermodynamic properties. However, not all approximants ($m>1$) for the correlation functions $\langle S_i^\alpha S_j^\alpha\rangle$ ($\alpha=x,y,z$) are invariant for the transformations mentioned above and therefore the results will depend on the choice of the decomposition.

C. Results

We now discuss some of the exact numerical results as obtained from RSD and CBD. In all our final computations we have taken $|J_1|=1$, $|J_3|=0,1$ and $h=0$.

In these units, $\beta=1$ corresponds to very low temperature as is seen from the small difference between the exact ground state energy and the exact thermal energy. To compare our results with those of [16], multiply our value of β with two. In Table 1, we

Table 1. The energy (specific heat) per site of a chain of 4 spins obtained from the approximants $Z_m^{\mathrm{RSD}}=Z_m^{\mathrm{CBD}}$ for the Heisenberg antiferromagnet ($J_1=J_3=-1$). The exact results for $m=\infty$ have been obtained by diagonalizing the full Hamiltonian. The column labelled by % denotes the percentage of non-zero terms in (2.5)

m	$\beta=0.25$	$\beta=0.5$	$\beta=1$	%
1	−0.676(0.187)	−1.384(0.616)	−2.094(0.593)	100
2	−0.644(0.163)	−1.198(0.445)	−1.807(0.826)	63
3	−0.638(0.159)	−1.156(0.393)	−1.652(0.656)	45
4	−0.636(0.157)	−1.140(0.373)	−1.583(0.539)	33
5	−0.635(0.156)	−1.133(0.364)	−1.549(0.473)	25
6	−0.634(0.156)	−1.129(0.358)	−1.529(0.434)	19
7	−0.634(0.155)	−1.126(0.355)	−1.517(0.409)	15
8	−0.634(0.155)	−1.125(0.353)	−1.510(0.393)	11
∞	−0.633(0.155)	−1.120(0.347)	−1.483(0.337)	

Table 2. The energy (specific heat) per site of a chain of 8 spins obtained from the approximant $Z_m^{\mathrm{RSD}}=Z_m^{\mathrm{CBD}}$ for the Heisenberg antiferromagnet ($J_1=J_3=-1$). The exact results for $m=\infty$ are obtained by diagonalizing the full Hamiltonian. A comparison with table 1 demonstrates that for fixed m the approximation becomes worse if the number of sites increases

m	$\beta=0.25$	$\beta=0.5$	$\beta=1$
1	−0.789(0.218)	−1.614(0.719)	−2.443(0.691)
2	−0.742(0.184)	−1.355(0.482)	−2.014(0.942)
3	−0.733(0.177)	−1.294(0.410)	−1.800(0.688)
∞	−0.726(0.172)	−1.242(0.345)	−1.565(0.251)

Table 3. Comparison between the correlation functions $\langle S_1^z S_3^z\rangle = \langle S_1^x S_3^x\rangle = \langle S_1^y S_3^y\rangle$ obtained from the RSD(CBD) in the case of the Heisenberg antiferromagnet ($N=7$)

m	$\beta=0.25$	$\beta=0.5$	$\beta=1$
1	0.090	0.378	0.866
2	0.067(0.068)	0.210(0.227)	0.388(0.547)
3	0.063(0.064)	0.185(0.194)	0.312(0.407)
∞	0.060	0.166	0.259

present the energy and specific heat per site for a system of 4 sites, $m=1,\ldots,8$ and $J_1=J_3=-1$. Both the energy and specific heat converge to their exact values. The energy converges monotonically and this trend has been found in all our calculations.

As could be expected, convergence is faster if β is small [11]. The rate of convergence also depends on the lattice size. In Table 2 we show the results for a chain of 8 sites. Fixing m and comparing the ratio's of the approximant to the exact results for different lattice sizes, we conclude that it is good practice to keep $\beta N/m$ constant if one wants to have equivalent approximants for all temperatures. Of course, the rate of convergence depends on the problem one is dealing with. For instance, we find that the approximants for the ferromagnet ($J_1=J_3=1$) are much better than for the XY-model ($J_1=1$, $J_3=0$) or antiferromagnet ($J_1=J_3=-1$).

This is related to the fact that in the simplest approximation ($m=1$), (2.5) only reproduces the correct ground state if $J_1=J_3=1$ [15].

In Table 3 we compare the correlation function $\langle S_1^x S_3^x\rangle=\langle S_1^y S_3^y\rangle=\langle S_1^z S_3^z\rangle$ as obtained from the RSD and CBD. Again we have chosen the antiferromagnet ($J_1=J_3=-1$). For $m=1$ both decompositions give the same results as can be seen from (2.5) and (2.8).

For low temperatures we find substantial disagreement between the different approaches. In general we observe that correlation functions calculated with the RSD decomposition converge faster than those obtained from the CBD.

This is easily understood because the CBD destroys the elementary property that the spin on site i is at the left of the spin on site $i+1$.

III. Periodic Boundary Conditions

A. Real Space Decomposition (RSD)

Here we use the same decomposition as in Sect. 2A. Because the calculation is almost identical with that of Sect. 2A, we just give the final result for the m-th approximant to the partition function

$$Z_m^{\mathrm{RSD}}=\sum_{\{\hat{S}_j\}}\sum_{\{S_{ij}\}}\prod_{j=1}^{m}\delta_{\phi_{Nj},1}\,T_{\hat{S}_j\phi_{1j}}(\hat{S}_{1j},\hat{S}_j\phi_{1j}S_{2j})$$
$$\cdot\,T_{\hat{S}_j\phi_{2j}}(\hat{S}_j\phi_{1j}S_{2j},\hat{S}_j\phi_{2j}S_{2j})$$
$$\ldots\,T_{\hat{S}_j\phi_{Nj}}(\hat{S}_j\phi_{N-1j}S_{Nj},S_{1j+1}). \tag{3.1}$$

This formula is very similar to (2.5) but the periodic boundary conditions introduce m additional degrees of freedom. Analytic results for $m=1$ can be found in [15] and Sect. 4. Because of the very nature of this partitioning of the Hamiltonian, translational invariance is broken. In general we observed that for all m the value of $\langle S_i^\alpha S_{i+n}^\alpha\rangle$ depends on whether or not i or $i+n$ equals 1 or N.

B. Path Sum Representation (PSR)

So far we have exploited the fact that it is easy to diagonalize a two-site problem. Here, we will decompose the hamiltonian into an XY-model and an Ising model. Because the eigenstates of the XY-model are known, we can find a representation for the m-th approximant to Z in terms of the (trivial) eigenstates of the Ising model

$$H_I = -J_3 \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z. \tag{3.2}$$

Thus we take $k=2$.

$$A_1 = -J_1 \sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y), \tag{3.3a}$$

$$A_2 = -J_3 \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^z, \tag{3.3b}$$

and we have

$$Z_m^{\mathrm{PSR}} \equiv \mathrm{Tr}\left[\exp\left(-\frac{\beta A_1}{m}\right)\exp\left(-\frac{\beta A_2}{m}\right)\right]^m. \tag{3.4}$$

Obviously, this representation yields exact results for all m if $J_1=0$ or $J_3=0$. It can be shown [12] that $Z_m^{\mathrm{PSR}} > Z$ and therefore we will obtain lower bounds for the free energy. If $J_1=J_3$, $h=0$ and m is finite, the operator

$$\left[\exp\left(-\frac{\beta A_1}{m}\right)\exp\left(-\frac{\beta A_2}{m}\right)\right]^m$$

does not have the same rotational symmetry as $\exp(-\beta H)$. The decomposition (3.4) breaks the rotational invariance around x or y-axis. However, rotation around the z-axis still is a symmetry operation and therefore the total magnetization M (given by $M=2p-N$ in the following) is still a good quantum number.

Thus we may write

$$Z_m^{\mathrm{PSR}} = \sum_{p=0}^{N} \exp[\beta h(2p-N)]\, Z_m(p) \tag{3.5a}$$

where

$$Z_m(p) = \mathrm{Tr}\left[\exp\left(-\frac{\beta A_1}{m}\right)\exp\left(-\frac{\beta H_I}{m}\right)\right]^m. \tag{3.5b}$$

In (3.5b) the trace is taken in the subspace of magnetization $M=2p-N$. We now proceed as in the case of the $1-d$ fermion model [4, 5].

We insert the eigenstates of the XY-Hamiltonian [17] between the two exponents in (3.5b) and evaluate the matrix elements.

We obtain

$$Z_m(p) = \exp[J_3(N-4p)] \sum_{\{n_{ij}\}} \prod_{j=1}^{M} \rho_j(\{n_{ij}\}) \tag{3.6a}$$

where

$$\rho_j(\{n_{ij}\}) = \exp\left[\frac{4\beta J_3}{m} \sum_{\lambda=1}^{p} \delta(|n_{\lambda,j+1} - n_{\lambda+1,j+1}| \bmod N - 1)\right] \cdot \left\{\sum_{P^{(j+1)}} \mathrm{sign}(P^{(j+1)}) \prod_{\lambda=1}^{p} I_p\left(\frac{4\beta J_1}{m}, n_{\lambda,j} - n_{P^{(j+1)}\lambda,j+1}\right)\right\}. \tag{3.6b}$$

Here the sites on which the p spins are up (or down) are denoted by $n_{\lambda,j}$, $\lambda=1,\ldots p$ and $P^{(j+1)}$ is a permutation operator acting on the label λ.

Formally, (3.6b) is the same as for the $1-d$ fermion model. There is however a slight difference. Here the functions I_p are given by

$$I_p(X,Y) = \frac{1}{N} \sum_{k \in K_p} \exp(X \cos k) \cos kY \tag{3.7a}$$

and

$$K_p = \begin{cases} \left\{0, \frac{2\pi}{N}, \ldots, \frac{2\pi(N-1)}{N}\right\} & \text{if } p \text{ is odd} \\ \left\{\frac{\pi}{N}, \frac{3\pi}{N}, \ldots, \frac{\pi(2N-1)}{N}\right\} & \text{if } p \text{ is even} \end{cases} \tag{3.7b}$$

whereas for the fermion problem

$$K_p = \left\{0, \frac{\pi}{N}, \frac{2\pi}{N}, \ldots, \frac{2\pi(N-1)}{N}\right\}.$$

From (3.6), one then derives expressions for the energy, specific heat and correlation functions of z-components of the spins. For the $(x-x)$-correlation functions one has to repeat the derivation because operators such as $S_1^x S_3^x + S_1^y S_3^y$ may modify a permutation operator.

C. Results

In Tables 4 and 5 we present the results for the energy and the specific heat per site for a system of 4 sites and $J_1=J_3=-1$, obtained from the RSD and PSR in the case of periodic boundary conditions. Because of the extra degrees of freedom in the RSD the computation time is considerably larger than for free boundary conditions and we were limited to $m=6$. For all temperatures we find good convergence but in general, the RSD converges faster than the PSR. This is quite opposite to the behavior found for the fermion model [5].

Table 4. The energy (specific heat) per site of a ring of 4 spins obtained from Z^{RSD} (periodic boundary conditions) for the Heisenberg antiferromagnet. The exact results for $m=\infty$ are obtained by diagonalizing the full Hamiltonian

m	$\beta=0.25$	$\beta=0.5$	$\beta=1$
1	−1.007(0.336)	−2.380(1.024)	−2.988(0.101)
2	−0.895(0.241)	−1.709(0.599)	−2.402(1.044)
3	−0.878(0.228)	−1.613(0.515)	−2.115(0.517)
4	−0.872(0.224)	−1.584(0.490)	−2.037(0.388)
5	−0.870(0.222)	−1.570(0.480)	−2.003(0.333)
6	−0.868(0.221)	−1.563(0.474)	−1.984(0.303)
∞	−0.865(0.218)	−1.548(0.462)	−1.944(0.232)

Table 5. The energy (specific heat) per site of a ring of 4 spins obtained from Z_m^{PSR} for the Heisenberg antiferromagnet. The exact results for $m=\infty$ are obtained by diagonalizing the full Hamiltonian. Comparison with Table 4 shows that the breaking of the $X-Y-Z$ symmetry has some influence on the rate of convergence (see also Table 6)

m	$\beta=0.25$	$\beta=0.5$	$\beta=1$
1	−0.921(0.259)	−1.827(0.666)	−2.366(0.243)
2	−0.881(0.231)	−1.661(0.587)	−2.247(0.451)
3	−0.873(0.224)	−1.604(0.531)	−2.142(0.474)
4	−0.869(0.222)	−1.581(0.504)	−2.076(0.431)
5	−0.868(0.221)	−1.569(0.490)	−2.036(0.385)
6	−0.867(0.220)	−1.563(0.481)	−2.011(0.350)
7	−0.867(0.220)	−1.559(0.476)	−1.994(0.325)
8	−0.866(0.219)	−1.556(0.473)	−1.983(0.305)
∞	−0.865(0.218)	−1.548(0.462)	−1.944(0.232)

Table 6. The ratio's $\langle S_q^z S_q^z\rangle/\langle S_q^x S_{-q}^x\rangle$ for $q=0(\pi)$ for a ring of 8 sites obtained from PSR in the case of the Heisenberg antiferromagnet. This representation destroys the equivalence between $X-Y$ and Z-components of the spins as is most clearly seen for $\beta=1$ and $q=0$

m	$\beta=0.25$	$\beta=0.5$	$\beta=1$
1	1.056(1.075)	2.774(1.455)	−0.066(2.495)
2	1.015(1.012)	1.237(1.132)	−0.031(1.645)
3	1.006(1.009)	1.099(1.061)	−1.223(1.344)
∞	1	1	1

Because the equivalence between X, Y and Z components is not broken in the RSD, this approach is expected to be more appropriate to the model than the PSR.

Symmetry considerations are very important in this approach to quantum statistical mechanics as is illustrated in Table 6. There we have given the ratio of the Fourier transformed correlation functions $\langle S_q^z S_{-q}^z\rangle_m$ and $\langle S_q^x S_{-q}^x\rangle_m$ for $q=0$, π, $N=8$ and $J_1=J_3=-1$.

For modest temperatures we find reasonable convergence but for low temperatures and $q=0$, there is no convergence at all. For ferromagnetic coupling $J_1=J_3=1$, our conclusions are roughly the same as in Sect. 2C, convergence thus being better.

IV. Analytic Results

In this section we give some analytic results for the RSD. The formulas presented here have been used as an independent check on our computer calculations.

First we take $m=1$. This special case has been investigated by Suzuki [16]. For free boundary conditions the partition function is given by

$$Z_1^{\mathrm{RSD}}=\sum_{\{S_i\}}\prod_{i=1}^{N} T_1(S_i,S_{i+1}) \tag{4.1}$$

and can be calculated by means of the transfer matrix technique. We obtain

$$Z_1^{\mathrm{RSD}}=\sum_{k=1}^{2}\gamma_k\lambda_k^N \tag{4.2a}$$

where

$$\lambda_k=\frac{a+d}{2}+(3-2k)\left[\left(\frac{a-d}{2}\right)^2+b^2\right]^{1/2} \tag{4.2b}$$

and

$$\gamma_k=(\lambda_k-a+b)^2/[(\lambda_k-a)^2+b^2]. \tag{4.2c}$$

In the thermodynamic limit, we obtain the following expressions for the correlation functions

$$\langle\sigma_i\rangle=[(\lambda_1-a)^2-b^2]/[(\lambda_1-a)^2+b^2] \tag{4.3a}$$

$$\langle\sigma_i^z\sigma_{i+n}^z\rangle-\langle\sigma_i^z\rangle^2=\frac{4b^4}{[(\lambda_1-a)^2+b^2][(\lambda_2-a)^2+b^2]}\left(\frac{\lambda_2}{\lambda_1}\right)^n \tag{4.3b}$$

$$\langle\sigma_i^x\sigma_{i+n}^x\rangle=(c/\lambda_1)^n. \tag{4.3c}$$

As could be expected for this quasi-classical approximation, the correlation functions (4.3b) and (4.3c) decay exponentially in space. In this crude approximation, the correlation length has an Ising-like temperature dependence.

For periodic boundary conditions one finds that $\langle S_1^\alpha S_{1+n}^\alpha\rangle+\langle S_2^\alpha S_{2+n}^\alpha\rangle$ if $n<N-1$. This demonstrates that the RSD breaks translational invariance.

One way to improve this approximation could be to keep $m=1$ and to decompose H by taking larger blocks

$$A_l=\sum_{i=(n-1)(l-1)+1}^{(n-1)l} H_{i,i+1} \tag{4.4}$$

where n denotes the number of spins in each block.

Then, it is possible to sum out the spins $S_{j'}$, $j'=(n-1)(l-1)+2,\ldots,(n-1)l-1$, $l=1,\ldots$ and still retain the formal expression (4.1) for the partition function.

However, this approach gives the same thermodynamic functions as obtained by diagonalizing one block and cannot be considered as a real improvement. Therefore the only way to improve the approximation is to increase m. For $m=2$ we may proceed as follows. First, we change variables by expressing S_{l2} in terms of $\phi_l\equiv\phi_{l1}=\phi_{l2}$ and $S_l\equiv S_{l1}$. We use the identity $\phi_{l-1}S_{l2}=\phi_l S_l$ and write the partition function in the form

$$Z_2^{\mathrm{RSD}} = \sum_{\{\phi_l\}} \delta_{\phi_{N+1\,1}} \cdot \sum_{\{S_l\}} \prod_{l=1}^{N} T_{\phi_l}(\phi_{l-1} S_l, \phi_l S_{l+1})\, T_{\phi_l}(\phi_l S_l, \phi_{l+1} S_{l+1}). \quad (4.5)$$

Let us now take $\phi_l = 1$; $l = 1, \ldots, N+1$. This configuration gives a contribution

$$a_1 = \sum_{\{S_l\}} \prod_{l=1}^{N} T_1^2(S_l, S_{l+1}), \quad (4.6)$$

which is easily worked out by means of the transfer matrix method. Let us now take $1 \leqq k \leqq N$ and $\phi_k = -1$. Because of (2.26) this leads to the condition $\phi_{k-1} = \phi_{k+1}$ and it follows that configurations of ϕ's where $\phi_i = \phi_{i+1} = -1$ do not contribute. For a given configuration of ϕ's one easily finds the contribution to the partition function but so far we have not been able to write down a simple analytic expression for $Z_2^{(1)}$ mainly because of the condition mentioned above.

V. Conclusions

We have investigated in detail some $2-d$ classical models equivalent to a $1-d$ spin-1/2 model. Our calculations demonstrate that in actual applications of the Trotter formula, it is essential that the approximants have the same symmetry properties as the original model system.

From our exact results we conclude that a good choice for the size of the lattice in the additional (Trotter) direction is determined by β and the lattice size of the quantum model.

In general, the convergence of the approximants is better for the Heisenberg ferromagnet than for the Heisenberg antiferromagnet or XY-model.

As already mentioned in the introduction, the ultimate goal is to study larger lattices than the ones studied in this paper. This can not be accomplished without some kind of importance sampling.

Although the equivalence with a $(d+1)$-dimensional classical model suggests that one may use standard Monte Carlo techniques [8], this is not the case. Several aspects are worth mentioning here. As can be seen in Table 1, a large number of configurations do not contribute to the partition function (2.5). Therefore additional algorithms to eliminate these configurations during the Monte Carlo process are required.

Because the magnetization is a conserved quantity, it is not possible to use a one-spin flip method [18]. General algorithms that change a few spins at a time [9, 19] become more complicated as m increases.

The most important problem is that it is very difficult to define a reasonable transition probability between states with different total magnetization.

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References

1. Suzuki, M.: Prog. Theor. Phys. **56**, 1454 (1976)
2. Barma, M., Shastry, B.S.: Phys. Rev. B**18**, 3351 (1978)
3. Barma, M., Shastry, B.S.: Phys. Lett. **61** A, 15 (1977)
4. De Raedt, H., Lagendijk, A.: Phys. Rev. Lett. **46**, 77 (1981)
5. De Raedt, H., Lagendijk, A.: J. Stat. Phys. (in press)
6. Hirsch, J.E., Scalapino, D.J., Sugar, R.L., Blankenbecler, R.: Phys. Rev. Lett. **47**, 1628 (1981)
7. Elliot, R.J., Pfeuty, P., Wood, C.: Phys. Rev. Lett. **25**, 443 (1970)
   Elliot, R.J., Wood, C.: J. Phys. C. **4**, 2359 (1971)
   Pfeuty, P., Elliot, R.J.: J. Phys. C. **4**, 2370 (1971)
8. Suzuki, M.: Prog. Theor. Phys. **46**, 1337 (1971)
9. Suzuki, M., Miyashita, S., Kuroda, A.: Prog. Theor. Phys. **58**, 1377 (1977)
10. Trotter, H.F.: Proc. Am. Math. Soc. **10**, 545 (1959)
11. Suzuki, M.: Comm. Math. Phys. **51**, 183 (1976)
12. Golden, S.: Phys. Rev. **137**, 1127 (1965)
    Lieb, E., Thirring, W.: Studies in Mathematical Physics. Princeton: Princeton University Press 1976
13. For a review see Bonner, J.C.: J. Appl. Phys. **49**, 1299 (1978)
14. Bonner, J.C.: In: Physics in one dimension. Edited by Bernasconi, J., Schneider, T. (ed.). Berlin, Heidelberg, New York: Springer Verlag 1981
15. Suzuki, M.: J. Phys. Soc. Jpn. **21**, 2274 (1966)
16. Bonner, J.C., Fisher, M.E.: Phys. Rev. B**5**, A 640 (1964)
17. Lieb, E., Schultz, T., Mattis, D.: Ann. Phys. **16**, 407 (1961)
18. Binder, K.: In: Phase transition and critical phenomena. Edited by Domb, C., Green, M.S. (eds.), Vol. 5b. London: Academic Press
19. Cullen, J.J., Landau, D.P.: Bull. Am. Phys. Soc. **576** (1981)

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